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PROBABILISTIC ANALYSIS BASED ON SIMULATIONS OF THE LONG-TERM GAS MIGRATION AT REPOSITORY-SCALE IN A GEOLOGICAL REPOSITORY FOR HIGH AND INTERMEDIATE LEVEL RADIOACTIVE WASTE DISPOSAL IN A DEEP CLAY FORMATION

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ABSTRACT

The current design for a deep geological repository for high- and intermediate-level radioactive waste in France consists of a complex system of different underground structures. In such a disposal system, some uncertainties related to physical parameters could arise from various origins. In the frame of the long-term performance assessment, probabilistic analysis must then be conducted to determine the physical parameters of the model, the uncertainty over which has a decisive influence on the general uncertainty concerning the long-term hydraulic evolution of the entire repository.

In that context, we conducted numerical simulations (using TOUGH2-MP) of an entire repository region, over a long-term period (up to 1 million years). However, such a detailed numerical model of the entire repository system requires a tremendous computational effort and poses a laborious task with respect to the operation of the model. To handle these difficulties, an innovative method for efficient numerical modeling of a complete repository system and its geologic environment has been applied (developed by AF-C for Andra and presented in the 2009 TOUGH Symposium). This method allows for a massive reduction in overall finite volume elements, while at the same time provides an adequate representation of the small-sized structures in the repository.

Using this method, probabilistic density functions (PDF) are defined for 10 physical parameters—including intrinsic permeabilities, capillary-pressure relationship parameters, porosities, diffusion coefficients, and corrosion rates. These distributions are then used to select 120 simulations using the Latin Hypercube Sampling (LHS) method. We then perform a statistical analysis, using relevant output results. This analysis consists of an uncertainty analysis (computation of quantiles, moments, distributions) and a sensitivity analysis (statistical-indicator calculations) whose objective is to rank the input parameters with respect to their importance to the hydraulic and gas transfer, and how they affect the output indicators. We thus identify those parameters that require better and more precise characterization.

INTRODUCTION

The French National Radioactive Waste Management Agency (Andra) have established the feasibility of a deep geological disposal of high-level and long-lived radioactivity waste in an argillaceous formation (Andra, 2005). The repository would be built within an indurated clay formation at around 500 m depth, and have a horizontal extension of roughly 3 km × 5 km. Questions related to the performance of this repository integrate concerns regarding the impact of the (mainly) hydrogen gas generated by anoxic corrosion of metallic components and radioactive waste. Of particular interest is the potential for overpressure in the near field of the repository, because this could affect the mechanical integrity of geotechnical and geologic barriers.

Achieving a good understanding of the hydraulic system behavior of the repository requires numerical, nonisothermal, two-phase flow and transport simulations. However, a detailed 3D modeling of the repository, accounting for both detailed structures at the local scale and the global geometry of the drift network, would require a tremendous computational effort, even when using a high-performance code like TOUGH2-MP (Zhang et al., 2008). To handle these difficulties, we developed an innovative method for the efficient numerical modeling of a complete repository system and its geologic environment (developed by AF-C for Andra and presented at the 2009 TOUGH Symposium). This method allows for a massive reduction in overall finite volume elements, while at the same time providing an adequate representation of the small-sized structures in the repository.

In such a disposal system, some uncertainties related to physical parameters could arise from various origins. In the frame of the long-term performance assessment, we must then conduct a probabilistic analysis.

This article describes a probabilistic study using hundreds of TOUGH2-MP simulations at global repository scale, in an attempt to determine the physical parameters of the model, the uncertainty over which has the greatest influence on the overall uncertainty of the entire repository's long-term hydraulic evolution.

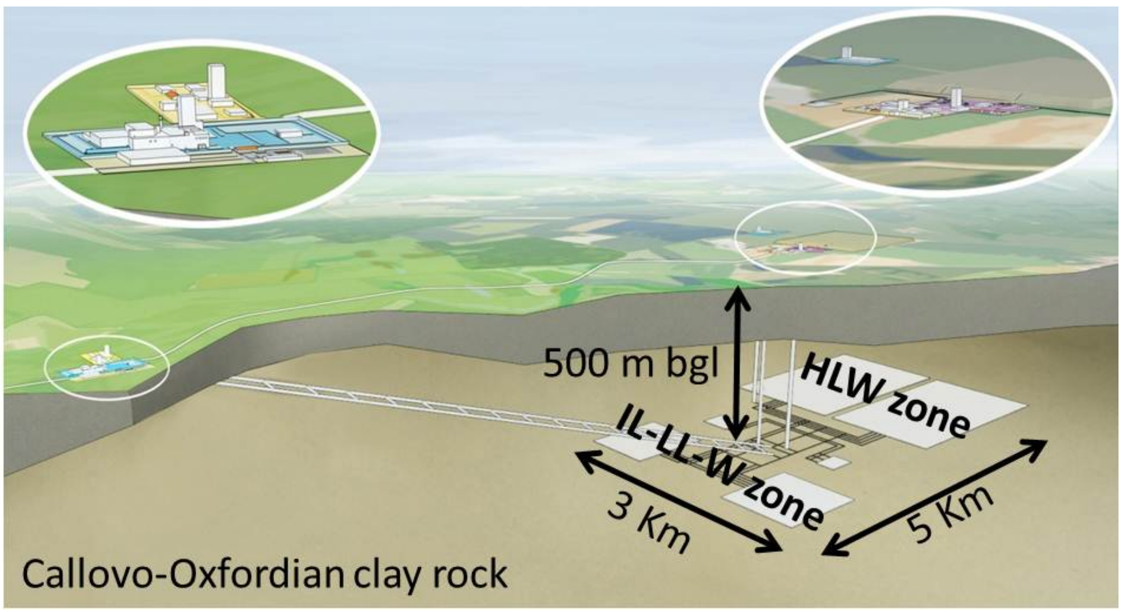

Figure 1. General architecture of the repository with emplacement of the HLW and ILW-LL zones

SYSTEM DESCRIPTION

The general layout of the repository is presented in **Figure 1**. The repository architecture is subdivided into three major zones: a large zone for high-level radioactive waste (HLW zone), a zone for long-lived intermediate-level radioactive waste (ILW-LL), and a zone for infrastructure facilities and access shafts in between. Inside the HLW zone, waste canisters are emplaced in several thousands of horizontal tunnels (0.75 m in diameter, 40 m long). In the ILW-LL zone, the waste canisters are emplaced in several tens of horizontal vaults (10 m in diameter, 400 m long). Individual wastes zones are connected through access and ventilation drifts. The horizontal extent of the complete repository is several kilometers in width and length; the thickness of the very-low-permeable host rock (Callovo-Oxfordian Clay) is around 150 m. The repository is located in the vertical mid-region of the host rock unit, around 500 m below ground level.

During the operational period of the repository (about 100 years), the complex network of drifts and disposal cells is ventilated under conditions of low relative humidity, leading to a drawdown of hydraulic pressure in the near field of the repository, as well as to a slight desaturation of the host rock in the vicinity of the drifts and caverns. At the end of the operational period, all repository structures are backfilled with specifically designed geomaterials. A set of hydraulic barriers (seals) is foreseen at the end of the emplacement drifts, at specific locations within and between the major zones, as well as in the upper part of the access shafts, to hinder the transport of potentially contaminated water or gas along the backfilled drifts and shafts.

During the post-operational period, the waste containers (in particular those with high-level waste) emit considerable amounts of heat, generated as a consequence of radioactive decay. Moreover, the corrosion and degradation of some waste components produce large amounts of gases (mostly hydrogen). Both processes have a strong impact on the resaturation of the repository and the geologic environment. The expected time scales of the major transient thermal and hydraulic phenomena is around 100,000 years

PHYSICAL PROCESSES

During the operational phase of the repository, the disposal and access drifts, as well as the access and ventilation shafts, are ventilated, and the low-permeable clay host rock is progressively depressurized and even desaturated in the vicinity of the drifts. The gas-water flow is modeled as two-phase flow using the generalized Darcy's law and the relative permeability/capillary pressure concept.

As soon as the drifts are backfilled and sealed, the post-operational period begins, and the principal processes modeled are:

- Thermal dissipation into the host rock, mainly by conduction, and an induced pore-water pressure increase by thermal expansion of the water[1].
- Resaturation of the backfill materials, due to the drainage towards the drifts and the capillary suction of the backfill materials (at early times)
- Hydrogen-gas generation and gas-pressure buildup in the backfilled repository[1].
- Displacement of water into the host rock due to the gas-pressure buildup[1].**Error! Reference source not found.Error! Reference source not found.Error! Reference source not found.**
- Dissolution of hydrogen into the pore water and transport by diffusion/advection[1].
- Advection and diffusion in the gas phase (in partially saturated backfill materials and host rock) and in the liquid (water) phase[1].

Because hydrogen is the dominant gas species, the TOUGH2-MP module EOS5 (water/hydrogen) is used for our computations (Pruess et al., 1999; Zhang et al., 2008). The impact of disregarding the true initial composition of the gas phase, e.g., air during the ventilation phase, is small on the scale of the entire repository and over the long term. Further, module EOS5 does not account for vapor-pressure lowering due to capillary and phase-adsorption effects. However, during the ventilation phase, the relative humidity prescribed at the surface of the drift walls is computed according to the vapor-pressure-lowering factor given by Kelvin's equation (cf. Pruess et al., 1999). Thus, the ventilation-driven desaturation of the porous waste containments, drift walls, and host rock is represented realistically. No geomechanical coupling is considered.

SPATIAL REPRESENTATION

A detailed numerical model of the entire repository system would require a tremendous computational effort and pose a laborious task with respect to the operation of the model. To offset this difficulty, an innovative method for the efficient numerical modeling of a complete repository system and its geologic environment has been applied (developed by AF-C for Andra and presented in the 2009 TOUGH symposium, Poller and al., 2009)—a method that allows for a massive reduction in overall finite volume elements, while at the same time providing an adequate representation of the small-sized structures in the repository.

This embedded modeling approach exploits the fact that, in the finite volume scheme, discretization does not necessarily need to respect spatially realistic geometries of the domain to be

[1] This process begins as soon as the waste packages are inserted into the emplacement drifts.

modeled. At first glance, this circumstance may seem irritating, but in view of the scale of the problem at hand, it offers the possibility for tackling the technical limitations inherent in the computation of large numerical models, and hence—important for this study—it paves the way for computation of the entire repository system with one single fully coupled model, including a physically and numerically appropriate representation of all spatial scales. This method enables us to keep the number of gridblocks for the designated model within a 100,000 magnitude (instead of a 10 million magnitude) for a complete repository representation. Schematically, and synthetically, the methodology considers three phases (Figure 2):

- Subdivision of the repository plane into a large number of "sectors" based on the position of seals and on geometrical considerations (e.g., different drift types or dimensions, symmetries). Each sector represents a 3D block of the geological pile (host rock and adjacent aquifers) and the repository components, such as access drifts, sealed drifts, and emplacement cells.
- A "multiplying concept" is used specifically for the approximation of symmetric[2] and repetitive structures, such as a series of emplacement cells along access drifts, as well as a series of waste emplacement areas. Thus, the number of gridblocks to be computed is reduced, while simultaneously the details of the geometrical fine-scale structures are accounted for. Several sectors are grouped to form a "zone" (e.g., a unit of high-level waste or a unit of intermediate level waste) by hydraulic connections at the drift interfaces.
- Interconnection of all zones at drift interfaces to form a model of the entire repository.

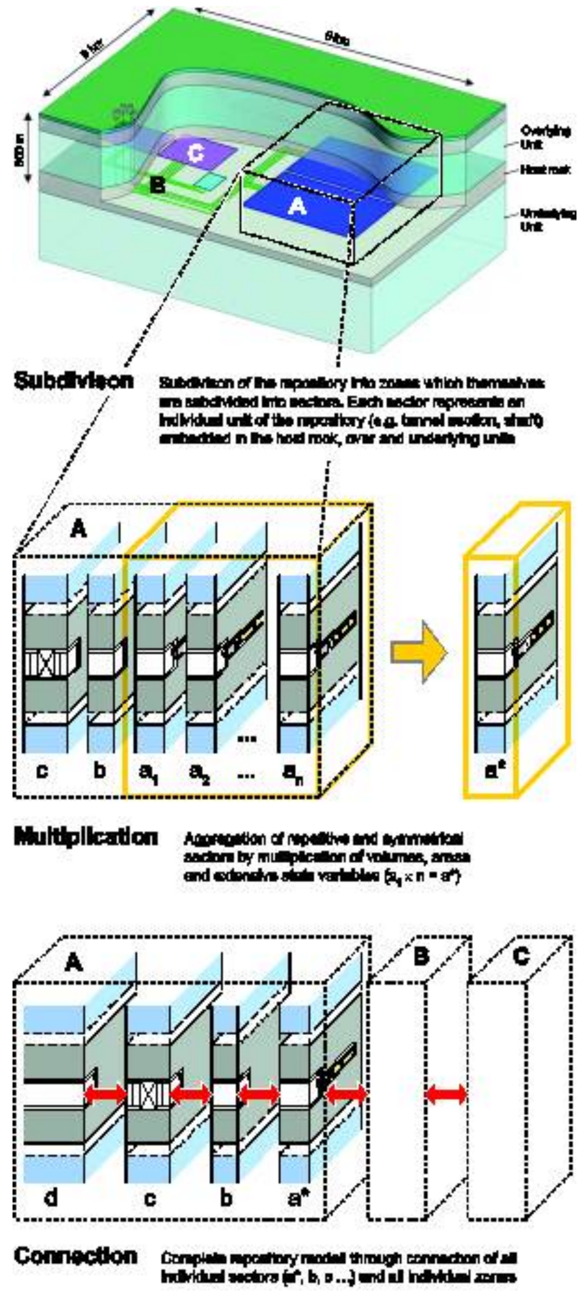

Figure 2. Schematic representation of the methodology used to develop the meshing

PARAMETERS

All parameter values were chosen to represent the available data. For some parameters however, the uncertainty is important, and the

[2] In this context symmetric conditions prevail if a spatially defined section of the repository (e.g. an emplacement cell with its surrounding host rock) appears in a repetitive manner, each section bearing identical conditions concerning its geometry, its hydraulic properties (materials, initial state, boundary conditions, sinks and sources). In other words, in every individual symmetric section, all conditions and processes influencing the thermo-hydraulics are identical in space and time.

presupposed influence on the simulation results is high. Simulations were done using a probabilistic approach for 10 of these parameters. Table 1 describes the way they were represented.

Table 1. Probabilistic Distribution Functions (PDF) for each parameter

	Type of PDF	Mean/SD	Min/Max
Host rock permeability (m/s)	Log Normal	$2\ 10^{-13}$ 10^{-13}	$10^{-14}/10^{-12}$
EDZ permeability (m/s)	Log Normal	10^{-9} $5\ 10^{-8}$	$10^{-11}/10^{-8}$
Bentonite permeability (m/s)	Log Uniform	-	$10^{-12}/10^{-10}$
Backfill porosity (%)	Uniform	-	20/50
Dissolved H2 molecular diffusion (m2/s)	Normal	$5\ 10^{-9}$ $2\ 10^{-9}$	$2\ 10^{-8}/10^{-9}$
VG-M n for EDZ (-)	Uniform	-	1.2/1.8
VG-M Pr for EDZ (MPa)	Uniform	-	0.5/10
VG-M n for bentonite (-)	Uniform	-	1.2/1.8
VG-M Pr for bentonite (MPa)	Uniform	-	1/15
Corrotion rate (micron/year)	Uniform	-	1/15

For permeability, Callovo-Oxfordian argilites and EDZ log-normal probabilistic functions were used, based on data for the mean, standard deviation, and minimum/maximum truncation values. For bentonite permeability, which can be conceptually designed, we assumed a uniform probabilistic function between acceptable values. Backfill porosity can also be designed, so the representation is the same as for bentonite permeability.

For dissolved H2 molecular diffusion literature **[?]** extreme values were chosen for minimum and maximum values, and normal probabilistic function assumed.

For van Genuchten/Mualem parameters (VG-M in the first column of **Table 1**) describing the unsaturated behavior of a porous media, we chose extreme values from partially available data and assumed uniform probabilistic distribution, owing to a lack of data regarding a more realistic distribution. For corrosion rate, extreme values were drawn from available data (on samples and *in situ* in the URL), and uniform distribution is assumed, again because of a lack of data regarding a more realistic distribution.

Figure 3 shows how the theoretical distributions are related by the actual 120 values chosen for dissolved H_2 molecular diffusion, corrosion rate, and EDZ permeability. All other parameters have been assigned values in line with the phenomenological knowledge concerning the process, mainly mean of available data for natural porous media and optimal designed values for engineered components.

These distributions are then used to construct 120 simulations via the LHS method. All these simulations were performed with TOUGH-MP software on highly parallel cluster Jade (more than 4 000 cores, property of the French CNRS organization). A total of 128 cores were used for each simulation, leading to a computation time of ~8 hours to one day to compute a 100,000 years two-phase flow period.

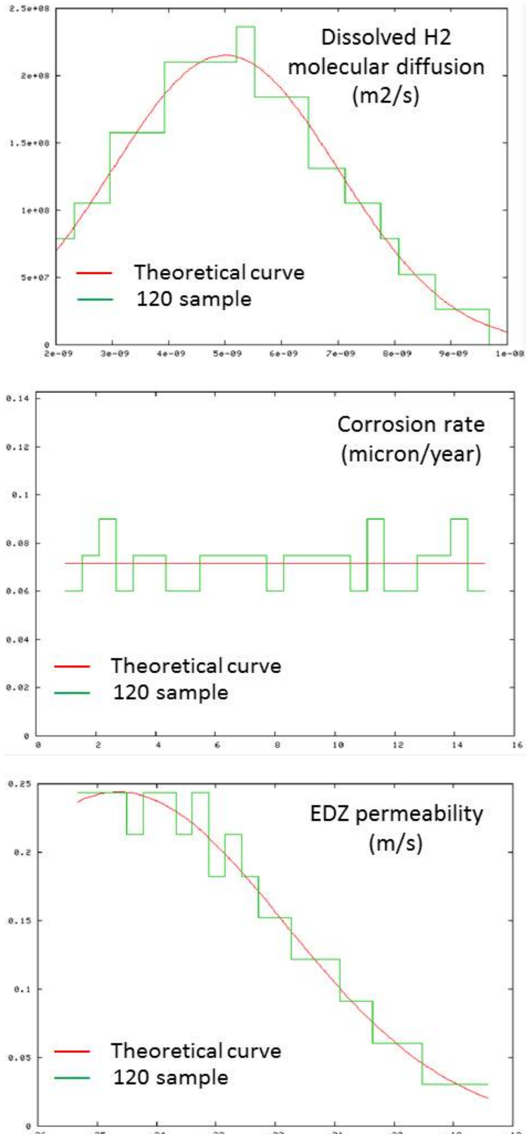

Figure 3. Theoretical and constructed PDF for selected parameters

MODELING RESULTS

The results presented here focus on one specific Andra concern, the eventual high gas pressures in the ILW-LL cells. figure 4 and figure 5 show several results for this state variable. The maximum is never higher than 5.5 MPa.

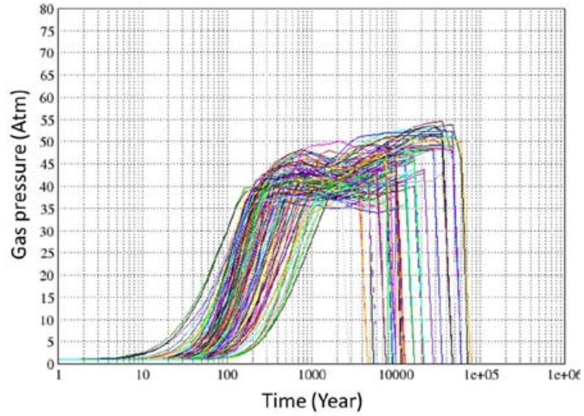

Figure 4. Calculated pressure in an ILW-LL vault for 120 simulations

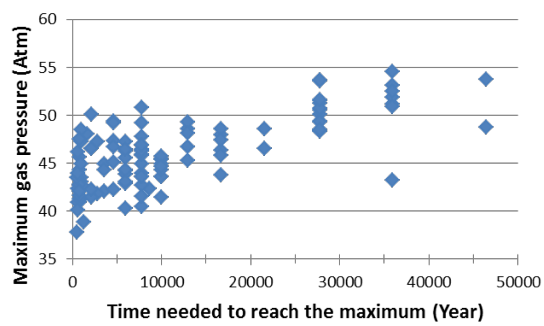

Figure 5. Maximum gas pressure for each simulation represented versus the time at which it appears

Depending on the simulation, this maximum occurs between several hundred years and several tens of thousands years. When occurring later, the maximum seems to be higher. This pressure is not a concern for the repository, since the hydrostatic water pressure is ~4.5 MPa, while the minimum mechanical stress at this depth is ~12 MPa.

The evolution of the maximum gas pressure as a function of the uncertain parameters allows us to define the first trend. We can see, in **figure 6**, a reasonable correlation between the solute molecular diffusion coefficient and the maximum gas pressure in the ILW-LL cells. Less significantly, corrosion rate and horizontal host-rock COX permeability seems to be correlated as well.

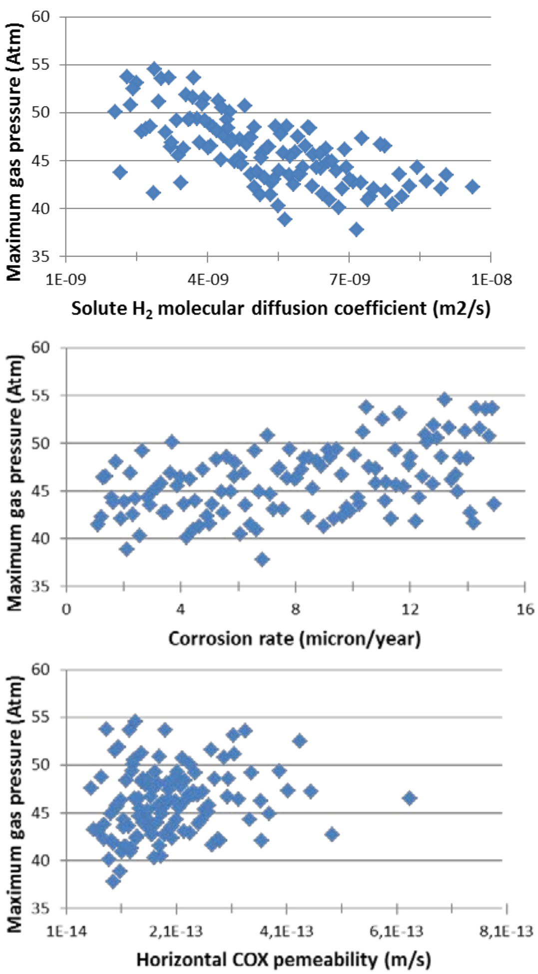

Figure 6. Maximum gas pressure for each simulation represented versus some chosen parameters values

To perform further statistical analyses we constructed a response surface based on a neural network, using URANY (Gaudier, 2008) and ROOT (Brun et al.) codes, combined with the 120 simulations described above. The determination coefficient between TOUGH results and response surface approximation shows a value greater than 0.95 (see figure 7)**,** which represents a first rough validation of this surface. To validate this surface more thoroughly, we generated several sets of entry (stochastic) parameters by the LHS method, including 1000, 2000, 5000, 10,000, 20,000, and 50,000 vectors and surface-based approximations for all these sets. Several statistical quantities (5% quintiles, 95% quintiles, mean, and median) were computed (see figure 8) showing a regularity of the surface when increasing the number of simulations in the set.

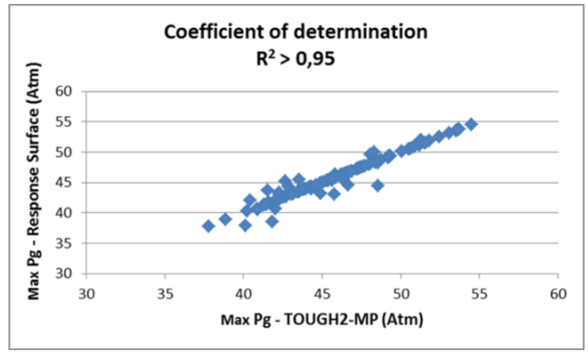

Figure 7. TOUGH vs. response surface results

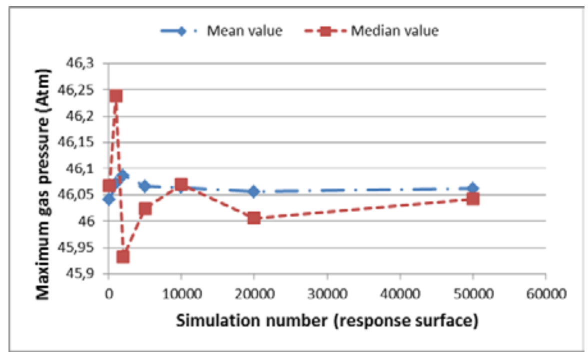

Figure 8. Evolution of maximum gas pressure mean and median values as a function of response-surface simulation results

Having shown that the surface is valid, we performed a sensitivity analysis to confirm the first correlation trend (figure 9).

The results show a consistency between several sensitivity estimators (PCC, Spearman, etc.) and also between the different simulation sets, from the initial 120-simulation set to the 50,000-simulation set.

The most influential parameter is the dissolved diffusion coefficient (on average, more than 50% of the gas dissolves inside the IL-LLW vaults); the second-most decisive parameter is the corrosion rate (the bigger the corrosion rate, the higher the gas pressure) and the third most decisive parameter is host-rock (COX) permeability (the higher the permeability, the higher the pressure). These findings highlight the fact that the water resaturating flux (which increases with this permeability) is an important variable controlling the gas pressure.

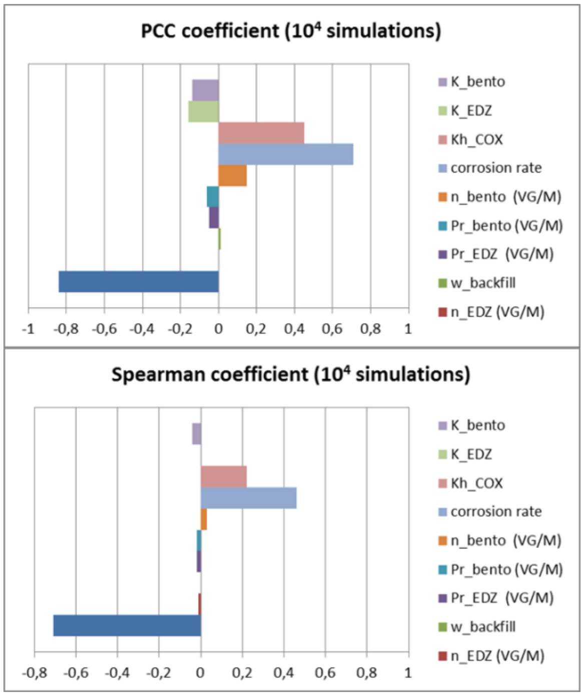

Figure 9. Sensitivity analysis results

FUTURE DIRECTIONS OF WORK

Our next step will be to add even more surface-response estimations, to reach a set large enough (at least 100,000 values) to perform a SOBOL analysis (sensitivity analysis on the variance, second-order statistical estimator) and to confirm the sensitivity analysis conducted up to now on the mean (first-order statistical estimator). Once this first methodological step is completed, we intend to do the same type of exercise on different criteria, including HLW maximum pressure, time of total resaturation of the repository, and maximum gas flux at the shafts.

Some parameters showing no impact on maximum pressure variance will be dropped from the stochastic analysis and replaced by others, like the Millington-Quirk exponent for saturation (linked to dissolved gas diffusion) or Henry's coefficient (linked to dissolution processes).

CONCLUSIONS

This first trial using TOUGH2-MP to generate hundreds of results at repository scale for the hydraulic-gas transient in a French nuclear repository, to define a surface response and statistical analysis, shows that this task is workable and the methodology well adapted. The "maximum pressure in ILW-LL vaults" criteria chosen for this first test shows that, for our concept, gas pressure is not an issue for this type of waste. The main parameters influencing this maximum gas pressure are the dissolved gas-diffusion coefficient, the corrosion rate, and the host-rock permeability.

Complementary work will be focused on more complex analysis like SOBOL estimators, use of new criteria (time of total resaturation, maximum gas flux through the shafts, etc.), and introducing new parameters in the statistical process.

ACKNOWLEDGMENT

K. Pruess (Lawrence Berkeley National Laboratory) is gratefully acknowledged for his help and for his insightful remarks in using TOUGH2. AF-C is acknowledged for its work done on the development of the embedded modeling approach and the generation of the entire process for launching a repository-scale simulation. CEA is acknowledged for granting the opportunity to use the URANY and ROOT codes to compute surface response and sensitivity analysis.

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